This is the accepted manuscript made available via CHORUS. The article has been published as:

Wu, Zhang, and Pantelides Reply:

Y.-N. Wu, X.-G. Zhang, and S. T. Pantelides

Phys. Rev. Lett. **120**, 039602 — Published 19 January 2018

DOI: 10.1103/PhysRevLett.120.039602

Wu, Zhang and Pantelides Reply

The Comment by Deng and Wei helps shed additional light on the issues that were covered in our Letter [1]. Here we recast their first point in order to bring out the fundamental differences between the conventional and the new approaches. We then examine their second point and show that the reported numerical results in fact strengthen the significance of the new approach advocated in our Letter [1].

In the conventional approach, charged point defects give rise to a divergence caused by the Coulombic tails of the defect potentials. The "jellium" potential is then introduced simply to remove the divergence in an *ad hoc* way. In light of our Letter, Deng and Wei interpret the jellium as a way to re-introduce the removed carriers in the system, rendering it neutral. The two approaches, however, are not equivalent in any sense. The jellium approach still remains at odds with statistical mechanics as the carriers are presumed to occupy a non-physical plane-wave state, whereas the rules of statistical mechanics prescribe that they occupy physical energy levels with true wave functions. Furthermore, the jellium leaves the Coulombic tails intact, whereas placing the carriers in physical states screens the Coulombic tails. This difference has implications on the resulting lattice relaxations [1]. Overall, the jellium approach can at best be described as an approximation to the true description derived in our Letter. It is, however, an uncontrolled approximation without any good justification for invoking it, as the full calculation is not more taxing computationally.

The second issue is the placement of the unbound carriers in the energy bands. In the calculations of Ref. [1], we placed the carriers in the energy bands of the supercell containing a defect, which is the correct way to do it. Those are the only physical states accessible to bound carriers, just as the electron in a free H atom is ionized into a Whittaker wave function, not a plane-wave state. The calculations reported by Deng and Wei highlight the significance of placing the carriers in the correct physical states as opposed to either perfect-crystal Bloch functions or a virtual plane-wave state at the Fermi energy as in the jellium scheme.

[1] Y.-N. Wu, X.-G. Zhang, and S. T. Pantelides, Phys. Rev. Lett. 119, 105501 (2017).